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Compact Gradient Tracking in Shape Optimization

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Abstract. In the present paper we consider the minimization of gradient tracking functionals defined on a compact and fixed subdomain of the domain of interest. The underlying state is assumed to satisfy a Poisson equation with Dirichlet boundary conditions. We prove that, in contrast to other type of objectives, defined on the whole domain, the shape Hessian is not strictly $H^{1/2}$-coercive at the optimal domain which implies ill-posedness of the shape problem under consideration.

Shape functional and gradient require only knowledge of the cauchy data of the state and its adjoint on the boundaries of the domain and the subdomain. These data can be computed in terms of boundary integral equations when reformulating the underlying differential equations as transmission problems. Thanks to fast boundary element techniques, we derive an efficient and accurate computation of the ingredients for optimization. Consequently, difficulties in the solution are related to the ill-posedness of the problem under consideration.

Introduction

Shape optimization is quite indispensable for designing and constructing industrial components. Many problems that arise in application, particularly in structural mechanics and in the optimal control of distributed parameter systems, can be formulated as the minimization of functionals defined over a class of admissible domains, see [17, 26, 29], and the references therein. Especially, the following situations are of interest. Namely, engineers aim in designing the shape of the domain $\Omega \in \mathbb{R}^n$ of definition for the underlying boundary value problem such that the state or its gradient achieves prescribed values in a fixed subregion $B \subset \Omega$. Mathematically speaking, this leads to an objective of the type

$$J(\Omega; u) := \int_B j\big(\mathbf{x}, u(\mathbf{x}), \nabla u(\mathbf{x})\big)\, d\mathbf{x} \to \inf$$

with the particular choices $j_1(u) = (u - u_d)^2$ or $j_2(u) = \|\nabla u - \nabla u_d\|^2$, where u_d is a given function. Principal studies for the solution of such problems can be found very often in literature, we refer e.g. to [26, 22] for a model problem in fluid flow and [15, 18, 20, 25] for optimization problems in magnetostatics. However, not much effort is spent on analyzing the nature of these problem type in more detail, for example by investigating the stability of stationary domains.

While analyzing the $L^2(B)$-tracking type objective j_1 in the foregoing paper [11], the aim of the present paper is to incorporate gradient values, i.e., investigating the prototype j_2. We use a boundary variational approach in combination with boundary integral representations to analyze the shape gradient and the shape Hessian. As an important result we prove the compactness of the shape Hessian for stationary domains. Since tracking type functionals allow a reinterpretation as inverse problems as well, see [1] for example, this refers to the ill-posedness of the underlying identification problem. We emphasize that these results remain valid even for arbitrary objectives of the type $j\big(\mathbf{x}, \nabla u(\mathbf{x})\big)$. Despite of a considerable progress in accuracy and efficiency of numerical methods, an oscillating behaviour of numerical solutions was observed for these class of problems. We are convinced that the lack of coercivity for compactly supported objectives is the main reason for the unsatisfactory behaviour of numerical algorithms.

Our numerical method adapts techniques from previous papers, see e.g. [9, 10], where we developed efficient algorithms for several elliptic shape optimization problems. Even in the case of compact gradient tracking functionals, all ingredients of the state equation that are required for the shape functional and its gradient, can be computed by boundary integral equations. Using a fast boundary element methods to solve the boundary integral equations, we gain a efficient and accurate method to compute the shape functional and its gradient. In particular, the use of boundary element methods requires only a discretization of the free boundary. To our opinion this is very advantageous since on the one hand, modern boundary element methods reduce the complexity compared to finite element methods, on the other hand, strong deformations of the domains are realizable without remeshing.

The authors like to point out that, in view of the above considerations, future research on appropriate regularization techniques is highly appreciated for the present class of problems. Here, appropriate means to find a compromise between regularizing in the spaces of natural coercivity of the underlying shape Hessian while providing numerical feasibility.

The paper is organized as follows. In Section 1 we introduce the second order shape calculus and analyze the problem under consideration. In particular, we prove that the Hessian of the shape functional is compact, which implies *ill-posedness* of the shape optimization problem. According to [12], we cannot expect convergence of a Ritz-Galerkin solution to the optimal domain since local strict convexity is missing. In Section 2 we consider the efficient solution of the state and its adjoint. We reformulate the underlying boundary value problems as boundary integral equations which are solved numerically by boundary element methods. We state error estimates concerning the proposed discretization. In Section 3, we carry out numerical tests which confirm that we succeeded in finding a fast method to solve the considered class of shape optimization problems. However, the results also indicate the ill-posedness of the optimization problem under consideration.

In the following, in order to avoid the repeated use of generic but unspecified constants, by $C \lesssim D$ we mean that C can be bounded by a multiple of D, independently of parameters which C and D may depend on. Obviously, $C \gtrsim D$ is defined as $D \lesssim C$, and $C \sim D$ as $C \lesssim D$ and $C \gtrsim D$.

1. Analyzing the Shape Optimization Problem

1.1. **Compact Gradient Tracking.** Let $\Omega \in \mathbb{R}^n$, $n = 2, 3$, be a simply connected domain with boundary $\Gamma := \partial\Omega$ and assume a compact set $B \subset \Omega$, see also Figure 1.1. The boundary of B will be denoted by $\Sigma := \partial B$. We shall consider the following shape

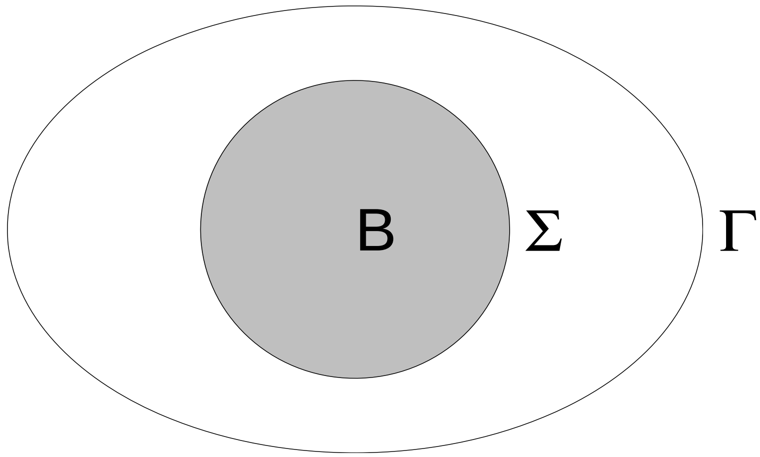

FIGURE 1.1. The domain Ω, the compact set B, and the boundaries Γ and Σ.

optimization problem

$$J(\Omega) = \frac{1}{2}\int_B \|\nabla u(\mathbf{x}) - \nabla u_d(\mathbf{x})\|^2 d\mathbf{x} \to \inf, \tag{1.1}$$

where the state u satisfies the boundary value problem

$$\begin{aligned} -\Delta u &= f \qquad \text{in } \Omega,\\ u &= g \qquad \text{on } \Gamma, \end{aligned} \tag{1.2}$$

and u_d is a given function. We suppose $u_d \in C^{2,\alpha}(B)$, $f \in C^{0,\alpha}(D)$, and $g \in C^{2,\alpha}(D)$ for some $\alpha \in (0,1)$, where $D \supset \Omega$ denotes the hold all. Notice that, since $B \subset\subset \Omega$ is assumed for all admissible domains Ω, the function u_d can be extended to $\widehat{u}_d \in C^{2,\alpha}(D)$ such that $\widehat{u}_d \equiv 0$ holds in a tubular neighbourhood $U_\delta(\Gamma)$ for some $\delta > 0$.

Following [7, 8] and denoting the outer normal at Γ (Σ) by $\mathbf{n}_\Gamma$ ($\mathbf{n}_\Sigma$), the directional derivative with respect to a sufficiently smooth domain or boundary perturbation field $\mathbf{V}$ reads as

$$\nabla J(\Omega)[\mathbf{V}] = \int_\Gamma \langle \mathbf{V}, \mathbf{n}_\Gamma \rangle \frac{\partial(g-u)}{\partial \mathbf{n}_\Gamma}\frac{\partial p}{\partial \mathbf{n}_\Gamma} d\sigma_{\mathbf{x}}. \tag{1.3}$$

Herein, the function p indicates the adjoint state. For $\mathbf{x}$ on Σ, let the notation

$$[f](\mathbf{x}) := \lim_{\substack{\mathbf{y}\to\mathbf{x}\\ \mathbf{y}\in B}} f(\mathbf{y}) - \lim_{\substack{\mathbf{y}\to\mathbf{x}\\ \mathbf{y}\in\Omega\setminus\overline{B}}} f(\mathbf{y}),$$

$$\left[\frac{\partial f}{\partial \mathbf{n}_\Sigma}\right](\mathbf{x}) := \lim_{\substack{\mathbf{y}\to\mathbf{x}\\ \mathbf{y}\in B}} \langle \nabla f(\mathbf{y}), \mathbf{n}_\Sigma(\mathbf{x})\rangle - \lim_{\substack{\mathbf{y}\to\mathbf{x}\\ \mathbf{y}\in\Omega\setminus\overline{B}}} \langle \nabla f(\mathbf{y}), \mathbf{n}_\Sigma(\mathbf{x})\rangle,$$

denote the jump of the Dirichlet and Neumann data of a function f at the boundary Σ. Then, p satisfies following transmission problem

$$\begin{aligned} -\Delta p &= f + \Delta u_d && \text{in } B, \\ [p] = 0, \quad \left[\frac{\partial p}{\partial \mathbf{n}_\Sigma}\right] &= \frac{\partial (u - u_d)}{\partial \mathbf{n}_\Sigma} && \text{on } \Sigma, \\ \Delta p &= 0 && \text{in } \Omega \setminus \overline{B}, \\ p &= 0 && \text{on } \Gamma. \end{aligned} \tag{1.4}$$

Of course, this is equivalent to (see Pironneau [26], for example)

$$\begin{aligned} -\Delta p &= \operatorname{div}\big(\chi_B \cdot \{\nabla u(\mathbf{x}) - \nabla u_d(\mathbf{x})\}\big) && \text{in } \Omega, \\ p &= 0 && \text{on } \Gamma, \end{aligned}$$

where χ_M is the characteristic function of a set M, i.e. $\chi_M = 1$ on M and $\chi_M = 0$ on $\mathbb{R}^n \setminus M$. Nevertheless, formulation (1.4) is more appropriate for a numerical solution via BEM.

1.2. **Shape Calculus.** In order to analyze the problem under consideration we have to look at the shape Hessian. Therefore, we require a second order shape calculus which we shall first focus on. The subsequent shape calculus, based on boundary variations, has been developed in [7, 8]. For a general overview on shape calculus, mainly based on the perturbation of identity (Murat and Simon) and the speed method (Sokolowski and Zolesio), we refer the reader for example to Murat and Simon [24, 28], Pironneau [26], Sokolowski and Zolesio [29], Delfour and Zolesio [6], and the references therein.

We introduce the following notation. The unit sphere in $\mathbb{R}^n$ will be denoted by

$$\mathbb{S} := \{\widehat{\mathbf{x}} \in \mathbb{R}^n : \|\widehat{\mathbf{x}}\| = 1\}.$$

Here and in the sequel, $\widehat{\mathbf{x}}$ indicates always a point on the unit sphere. In particular, for a point $\mathbf{x} \in \mathbb{R}^n$ the notion $\widehat{\mathbf{x}}$ has to be understood as $\widehat{\mathbf{x}} := \mathbf{x}/\|\mathbf{x}\|$.

We have to assume $\Omega \in C^{2,\alpha}$ for some fixed $\alpha \in (0,1)$ for the second order boundary perturbation calculus, in contrast to $\Omega \in C^2$ for the first order calculus. For sake of simplicity, we suppose the domain Ω to be star-shaped. Then, we can identify it with a function, that describes its boundary in accordance with $\Gamma = \{r(\widehat{\mathbf{x}}) \cdot \widehat{\mathbf{x}} : \widehat{\mathbf{x}} \in \mathbb{S}\}$, where $r \in C^{2,\alpha}(\mathbb{S})$ is a positive function with $r \geq \delta > 0$. We consider functions $dr \in C^{2,\alpha}(\mathbb{S})$ as standard variation for perturbed domains Ω_ε and boundaries Γ_ε, respectively, defined via $r_\varepsilon(\widehat{\mathbf{x}}) = r(\widehat{\mathbf{x}}) + \varepsilon dr(\widehat{\mathbf{x}})$. The main advantage of the present approach is a complete embedding of the shape problem into a Banach space setting. That is, both, the shapes and their increments, can be viewed as elements of $C^{2,\alpha}(\mathbb{S})$.

In accordance with the previous subsection, we find for our particular setting the identities $\mathbf{V}(\mathbf{x}) = dr(\widehat{\mathbf{x}}) \cdot \widehat{\mathbf{x}}$ and

$$\langle \mathbf{V}, \mathbf{n}_\Gamma \rangle d\sigma_{\mathbf{x}} = dr(\widehat{\mathbf{x}})\langle \widehat{\mathbf{x}}, \mathbf{n}_\Gamma \rangle d\sigma_{\mathbf{x}} = dr(\widehat{\mathbf{x}}) r(\widehat{\mathbf{x}})^{n-1} d\sigma_{\widehat{\mathbf{x}}} \tag{1.5}$$

for all $\mathbf{x} \in \Gamma$. Consequently, the shape gradient (1.3) becomes in spherical coordinates

$$\nabla J(\Omega)[dr] = \int_{\mathbb{S}} dr\, r^{n-1} \frac{\partial p}{\partial \mathbf{n}_\Gamma} \frac{\partial (g-u)}{\partial \mathbf{n}_\Gamma} d\sigma. \tag{1.6}$$

The shape Hessian defines a continuous bilinear form on $H^{1/2}(\Gamma) \times H^{1/2}(\Gamma)$, namely

$$\begin{aligned} \nabla^2 J(\Omega)[dr_1, dr_2] = \int_{\mathbb{S}} dr_1 dr_2 \bigg\{ (n-1) r^{n-2} \frac{\partial p}{\partial \mathbf{n}_\Gamma} \frac{\partial (g-u)}{\partial \mathbf{n}_\Gamma} + r^{n-1} \frac{\partial}{\partial \widehat{\mathbf{x}}} \Big[\frac{\partial p}{\partial \mathbf{n}_\Gamma} \cdot \frac{\partial (g-u)}{\partial \mathbf{n}_\Gamma} \Big] \bigg\} \\ + r^{n-1}\, dr_1 \Big[\frac{\partial dp[dr_2]}{\partial \mathbf{n}_\Gamma} \cdot \frac{\partial (g-u)}{\partial \mathbf{n}_\Gamma} - \frac{\partial p}{\partial \mathbf{n}_\Gamma} \cdot \frac{\partial du[dr_2]}{\partial \mathbf{n}_\Gamma} \Big] d\sigma, \end{aligned} \tag{1.7}$$

cf. [7, 8]. Herein, the notion $\partial/\partial \widehat{\mathbf{x}}$ has to be understood in the sense of $\partial u/\partial \widehat{\mathbf{x}} = \langle \nabla u, \widehat{\mathbf{x}} \rangle$. Moreover, $du = du[dr_2]$ and $dp = dp[dr_2]$ denote the local shape derivatives of the state and its adjoint, that satisfy the boundary value problems

$$\begin{aligned} \Delta du &= 0 && \text{in } \Omega, \\ du &= dr_2 \langle \widehat{\mathbf{x}}, \mathbf{n} \rangle \frac{\partial (g-u)}{\partial \mathbf{n}_\Gamma} && \text{on } \Gamma, \end{aligned} \tag{1.8}$$

and

$$\begin{aligned} \Delta dp &= 0 && \text{in } \Omega \setminus \Sigma, \\ [dp] = 0, \quad \left[\frac{\partial dp}{\partial \mathbf{n}_\Sigma} \right] &= \frac{\partial du[dr_2]}{\partial \mathbf{n}_\Sigma} && \text{on } \Sigma, \\ dp &= -dr_2 \langle \widehat{\mathbf{x}}, \mathbf{n}_\Gamma \rangle \frac{\partial p}{\partial \mathbf{n}_\Gamma} && \text{on } \Gamma. \end{aligned} \tag{1.9}$$

Remark 1.1. *Equivalent domain integral representations for the shape gradient and shape Hessian can be directly derived from the differentiation of* (1.1). *We have*

$$\begin{aligned} \nabla J(\Omega)[dr] &= \int_B \langle \nabla \big(u - u_d\big)(\mathbf{x}), \nabla du[dr](\mathbf{x}) \rangle d\mathbf{x}, \\ \nabla^2 J(\Omega)[dr_1, dr_2] &= \int_B \langle \nabla du[dr_1], \nabla du[dr_2] \rangle + \langle \nabla (u - u_d), \nabla du^2[dr_1, dr_2] \rangle d\mathbf{x}, \end{aligned} \tag{1.10}$$

where the second local derivative $d^2 u = d^2 u[dr_1, dr_2]$ of the state u satisfies a characterization equation similar to the first derivative

$$\begin{aligned} \Delta d^2 u &= 0 && \textit{in } \Omega, \\ d^2 u &= dr_1 dr_2 \frac{\partial^2 (g-u)}{\partial \widehat{\mathbf{x}}^2} - dr_1 \frac{\partial du[dr_2]}{\partial \widehat{\mathbf{x}}} - dr_2 \frac{\partial du[dr_1]}{\partial \widehat{\mathbf{x}}} && \textit{on } \Gamma, \end{aligned} \tag{1.11}$$

see [7] *for the details. Especially, symmetry of the shape Hessian is obvious.*

1.3. **Compactness of the Hessian at the Optimal Domain.** Next, we will investigate the shape Hessian at a stationary domain $\Omega^\star$, that is, the first order necessary condition $\nabla J(\Omega^\star)[dr] = 0$ holds for all $dr \in C^{2,\alpha}(\mathbb{S})$. Consequently, all quantities arising in the considerations below are related to the domain $\Omega^\star$. Notice that the necessary condition implies

$$\frac{\partial p}{\partial \mathbf{n}_\Gamma}\frac{\partial(u-g)}{\partial \mathbf{n}_\Gamma} \equiv 0 \quad \text{on } \Gamma. \tag{1.12}$$

Lemma 1.2. *Equation* (1.12) *is satisfied if and only if* $\partial(u-g)/\partial\mathbf{n}_\Gamma \equiv 0$ *on* Γ *or* $\partial p/\partial\mathbf{n}_\Gamma \equiv 0$ *on a subset* $\Phi \subset \Gamma$ *with positive measure relative to* Γ. *In the latter case it follows* $p \equiv 0$ *in* $\Omega^\star \setminus \overline{B}$.

Proof. Assume the $\partial p/\partial\mathbf{n}_\Gamma \equiv 0$ on a subset $\Phi \subset \Gamma$ with nontrivial measure. Then, since p is harmonic in $\Omega^\star \setminus \overline{B}$ according to (1.4) and due to the homogeneous Dirichlet boundary conditions at Γ, the unique continuation property for C^2-boundaries (cf. Hörmander [19]) implies immediately the assertion. □

The solution $\partial(u-g)/\partial\mathbf{n}_\Gamma \equiv 0$ corresponds to a degeneration of the data or of the whole shape problem, respectively, and makes no sense. In particular, it would imply $du[dr] \equiv 0$ for all admissible dr, see (1.8). Thus, we suppose $\partial p/\partial\mathbf{n}_\Gamma \equiv 0$. Then, since $p \equiv 0$ in $\Omega^\star \setminus B$ according to Lemma 1.2, the shape Hessian simplifies to

$$\nabla^2 J(\Omega^\star)[dr_1, dr_2] = \int_{\mathbb{S}} r^{n-1}\, dr_1 \frac{\partial dp[dr_2]}{\partial \mathbf{n}_\Gamma} \cdot \frac{\partial(g-u)}{\partial \mathbf{n}_\Gamma}\, d\sigma. \tag{1.13}$$

Notice that the adjoint local shape derivative $dp = dp[dr]$ (1.9) admits homogeneous boundary conditions at Γ. Consequently, employing the fundamental solution $E(\mathbf{x},\mathbf{y})$ of the Laplacian, given by

$$E(\mathbf{x},\mathbf{y}) = \begin{cases} -\frac{1}{2\pi}\log\|\mathbf{x}-\mathbf{y}\|, & \text{if } n=2,\\ \frac{1}{4\pi\|\mathbf{x}-\mathbf{y}\|}, & \text{if } n=3, \end{cases} \tag{1.14}$$

the adjoint local shape derivative dp satisfies

$$dp(\mathbf{x}) = \int_\Sigma E(\mathbf{x},\mathbf{y})\frac{\partial du}{\partial \mathbf{n}_\Sigma}(\mathbf{y})\, d\sigma_{\mathbf{y}}, \qquad \mathbf{x} \in \Omega^\star. \tag{1.15}$$

The next result is derived as an immediate consequence of the identities (1.10).

Lemma 1.3. *Suppose* $\partial(u-g)/\partial\mathbf{n}_\Gamma \neq 0$ *almost everywhere on* Γ. *Moreover, we suppose that the exceptional direction* $dr^\star$, *defined by*

$$dr^\star(\widehat{\mathbf{x}}) = \frac{1}{r(\widehat{\mathbf{x}})\cdot \frac{\partial(g-u)}{\partial \mathbf{n}_\Gamma}(\widehat{\mathbf{x}})}, \quad \widehat{\mathbf{x}} \in \mathbb{S}, \tag{1.16}$$

is not admissible, that is $dr^\star \notin H^{1/2}(\Gamma)$. *Then, the shape Hessian* $\nabla^2 J(\Omega^\star)$ *is a positive bilinear form on* $H^{1/2}(\Gamma) \times H^{1/2}(\Gamma)$, *i.e.*,

$$\nabla^2 J(\Omega^\star)[dr, dr] > 0$$

for all $dr \not\equiv 0$.

Proof. We show first that the second term of the domain representation of the shape Hessian in (1.10) vanishes at $\Omega^\star$, that is

$$\int_B \langle \nabla(u-u_d)(\mathbf{x}), \nabla d^2u[dr,dr](\mathbf{x})\rangle\, d\mathbf{x} = 0, \tag{1.17}$$

for all admissible dr. Using (1.4), the following transform is obvious

$$\begin{aligned}\int_B \langle \nabla(u-u_d), \nabla d^2u[dr,dr]\rangle d\mathbf{x} &= \int_{\Omega^\star} \langle \nabla p, \nabla d^2u[dr,dr](\mathbf{x})\rangle d\mathbf{x}\\ &= \int_\Gamma \frac{\partial d^2u[dr,dr]}{\partial \mathbf{n}} p(\mathbf{x})\, d\sigma_{\mathbf{x}}.\end{aligned}$$

Hence, (1.17) follows immediately from (1.4). Consequently, we arrive at the identity

$$\nabla^2 J(\Omega^\star)[dr,dr] = \int_B \|\nabla du[dr](\mathbf{x})\|^2\, d\mathbf{x}.$$

Observing that $du[dr]$ is harmonic, we conclude that $du[dr] \neq const.$ almost everywhere on B provided that $dr \not\equiv dr^\star$ and $dr \not\equiv 0$. This implies the assertion. □

Note that, if $dr^\star$ is admissible, there holds $du[dr^\star] \equiv const.$ and consequently $\nabla^2 J(\Omega^\star)[dr^\star, dr^\star] = 0$ due to $\nabla du[dr^\star] \equiv 0$. Especially, if $\partial(g-u)/\partial\mathbf{n}_\Gamma \in C^{2,\alpha}(\Gamma)$ is strictly positive or negative, $dr^\star$ defines a regular perturbation for $\Omega^\star$ with vanishing second variation with respect to the objective. Therefore, there may exist a connected family of stationary domains, as it is illustrated by the following example.

Example 1.4. *We denote by*

$$B_z := \{(x,y) \in \mathbb{R}^2 : x^2 + y^2 < z^2\}, \quad z > 0,$$

the ball with radius z. We consider $B := B_1$, $u_d \equiv 0$, $g \equiv 0$ and $f \equiv 4$. As one readily verifies, the state with respect to the domain B_z ($z > 1$) is given by $u(B_z) = z^2 - (x^2+y^2)$. According to (1.4), the adjoint state $p(B_z)$ is given as

$$p(B_z; x, y) = \begin{cases} 1-(x^2+y^2), & \text{if } x^2+y^2 \le 1,\\ 0, & \text{if } 1 < x^2+y^2 \le z.\end{cases}$$

Consequently, any domain B_z is a stationary domain and obviously $J(B_{z_1}) = J(B_{z_2})$ for arbitrary $z_2 > z_1 > 1$. The direction $dr^\star \equiv const.$, corresponding to the direction of blowing up or shrinking the circle, refers to this degeneration.

We emphasize again that the domain $\Omega^\star$ is only a regular strict minimizer of second order if the shape Hessian is *strictly* $H^{1/2}(\Gamma)$-coercive, that is $\nabla^2 J(\Omega^\star)[dr,dr] \gtrsim \|dr\|^2_{H^{1/2}(\Gamma)}$, cf. [2, 3, 12]. We will show next that the shape Hessian is compact which immediately implies that strict $H^{1/2}(\Gamma)$-coercivity can never be satisfied, independent of wether the exceptional direction $dr^\star$ exists or not.

Lemma 1.5. *Assume $u, g \in C^{2,\alpha}(\Gamma)$, then the multiplication operator*

$$M : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma), \qquad M dr := dr \cdot \langle \widehat{\mathbf{x}}, \mathbf{n} \rangle \frac{\partial (g-u)}{\partial \mathbf{n}} \tag{1.18}$$

is continuous.

Proof. Abbreviating $\omega := \langle \widehat{\mathbf{x}}, \mathbf{n}_\Gamma \rangle \partial(g-u)/\partial \mathbf{n}$ we may write $M dr = dr \cdot \omega$. Due to results of Triebel [30] or Mazja and Shaposhnikova [21], the multiplication operator M is continuous from $H^{1/2}(\Gamma)$ to $H^{1/2}(\Gamma)$, since $\omega \in C^{0,\alpha}(\Gamma)$ for some $\alpha > 1/2$. □

Lemma 1.6. *The mapping*

$$\Lambda : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma), \quad \Lambda(M dr) = \frac{\partial dp[dr]}{\partial \mathbf{n}},$$

that maps $M dr \in H^{1/2}(\Gamma)$ via (1.8) and (1.15) onto the Neumann data $\partial dp[dr]/\partial \mathbf{n} \in H^{-1/2}(\Gamma)$ of the adjoint local shape derivative, is compact.

Proof. It is well known, that the Dirichlet-to-Neumann map $\mathcal{A} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ maps the given Dirichlet data $du[dr]|_\Gamma = M dr \in H^{1/2}(\Gamma)$ continuously to the Neumann data $\partial du[dr]/\partial \mathbf{n} = \mathcal{A}(M dr) \in H^{-1/2}(\Gamma)$. Green's representation formula yields

$$du[dr](\mathbf{x}) = \int_\Gamma E(\mathbf{x}, \mathbf{y}) \frac{\partial du[dr]}{\partial \mathbf{n}_\Gamma}(\mathbf{y}) d\sigma_\mathbf{y} - \int_\Gamma \frac{\partial E(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_\Gamma(\mathbf{y})} du[dr](\mathbf{y}) d\sigma_\mathbf{y}, \quad \mathbf{x} \in \Omega^\star,$$

with $E(\mathbf{x}, \mathbf{y})$ given by (1.14). Since $\operatorname{dist}(\mathbf{B}, \Gamma) > 0$, one readily infers that differentiation gives

$$\nabla du[dr](\mathbf{x}) = \int_\Gamma \nabla_\mathbf{x} E(\mathbf{x}, \mathbf{y}) \frac{\partial du[dr]}{\partial \mathbf{n}_\Gamma}(\mathbf{y}) d\sigma_\mathbf{y} - \int_\Gamma \nabla_\mathbf{x} \frac{\partial E(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_\Gamma(\mathbf{y})} du[dr](\mathbf{y}) d\sigma_\mathbf{y},$$

where the kernels $\nabla_\mathbf{x} E(\mathbf{x}, \cdot)$ and $\nabla_\mathbf{x} \partial E(\mathbf{x}, \cdot)/\partial \mathbf{n}_\Gamma(\cdot)$ keep still bounded in $[H^{1/2}(\Gamma)]^n$ and $[H^{-1/2}(\Gamma)]^n$ for all $\mathbf{x}$ on Σ, respectively. Hence we arrive at

$$\begin{aligned} \left\| \frac{\partial du}{\partial \mathbf{n}_\Sigma} \right\|_{H^{-1/2}(\Sigma)} &\le \max_{\mathbf{x} \in \mathbf{\Sigma}} \| \nabla_\mathbf{x} E(\mathbf{x}, \cdot) \|_{[H^{1/2}(\Gamma)]^n} \| \mathcal{A}(M dr) \|_{H^{-1/2}(\Gamma)} \\ &\qquad + \max_{\mathbf{x} \in \mathbf{\Sigma}} \left\| \nabla_\mathbf{x} \frac{\partial E(\mathbf{x}, \cdot)}{\partial \mathbf{n}_\Gamma(\cdot)} \right\|_{[H^{-1/2}(\Gamma)]^n} \| M dr \|_{H^{1/2}(\Gamma)} \\ &\lesssim \| M dr \|_{H^{1/2}(\Gamma)}, \end{aligned}$$

which implies the continuity of

$$\mathcal{B} : H^{1/2}(\Gamma) \to H^{-1/2}(\Sigma), \quad \mathcal{B}(M dr) = \frac{\partial du}{\partial \mathbf{n}_\Sigma}.$$

Next, we notice that the mapping

$$\mathcal{C} : H^{-1/2}(\Sigma) \to H^{-1/2}(\Gamma), \quad (\mathcal{C} f)(\mathbf{x}) = \int_\Sigma \frac{\partial E(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_\Gamma(\mathbf{x})} f(\mathbf{y}) d\sigma_\mathbf{y},$$

is compact. Consequently, in view of (1.15), since the Neumann data of the adjoint local shape derivative are computed by

$$\frac{\partial dp}{\partial \mathbf{n}_\Gamma} = (\mathcal{C} \circ \mathcal{B})(M dr),$$

we obtain the desired assertion. $\square$

Obviously, the shape Hessian (1.13) defines a continuous bilinear form on $H^{1/2}(\Gamma) \times H^{1/2}(\Gamma)$, namely

$$\nabla^2 J(\Omega^\star)[dr_1, dr_2] = \big(M dr_1, \Lambda(M dr_2)\big)_{L^2(\Gamma)}. \tag{1.19}$$

According to the Lemmata 1.5 and 1.6 we conclude the final result.

Proposition 1.7. *The shape Hessian*

$$\mathcal{H} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma), \quad \mathcal{H} = 2M^\star \Lambda M : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma),$$

is compact at the optimal domain $\Omega^\star$*.*

Remark 1.8. *Assuming the boundary* Γ *to be arbitrarily smooth, one readily infers that the shape Hessian is even compact as a mapping* $\mathcal{H} : H^s(\Gamma) \to H^{-s}(\Gamma)$ *for all* $s > 1/2$*.*

This proposition implies the ill-posedness of the optimization problem itself, which is completely characterized by the nature of the shape Hessian at the critical domain.

1.4. **Ritz-Galerkin Approximation of the Shape Problem.** In order to solve the minimization problem defined by (1.1) and (1.2), we are looking for the stationary points $\Omega^\star$ satisfying

$$\nabla J(\Omega^\star)[dr] = 0 \quad \text{for all } dr \in C^{2,\alpha}(\mathbb{S}). \tag{1.20}$$

In accordance with [12] we shall introduce a Ritz-Galerkin method for the nonlinear equation (1.20). To this end, we restrict ourselves again to star-shaped domains and consider the gradient in terms of sphericals coordinates (1.6). Nevertheless, one can consider any fixed variation field with respect to a smooth reference manifold as well, see [12] for the details.

Let $\phi_1, \phi_2, \ldots, \phi_N$ denote the first N spherical harmonics in $\mathbb{R}^n$ and consider the ansatz space

$$V_N = \operatorname{span}\{\phi_1, \phi_2, \ldots, \phi_N\} \subset C^{2,\alpha}(\mathbb{S}).$$

Identifying the (finite dimensional) domain Ω_N and the radial function

$$r_N(\widehat{\mathbf{x}}) = \sum_{n=0}^{N} a_n \phi_n(\widehat{\mathbf{x}}), \quad \widehat{\mathbf{x}} \in \mathbb{S},$$

we can replace (1.20) by its finite dimensional counterpart:

$$\text{seek } r_N^\star \in V_N \text{ such that} \quad \nabla J(r_N^\star)[dr] = 0 \quad \text{for all } dr \in V_N. \tag{1.21}$$

Note that this is the necessary condition associated with the finite dimensional optimization problem

$$J(r_N) \to \min, \quad r_N \in V_N. \tag{1.22}$$

According to [12] we obtain an approximation error that stays in the energy norm $H^{1/2}(\mathbb{S})$ proportional to the best approximation in V_N, that is

$$\|r_N^\star - r^\star\|_{H^{1/2}(\mathbb{S})} \lesssim \inf_{r_N \in V_N} \|r_N - r^\star\|_{H^{1/2}(\mathbb{S})},$$

provided that the shape Hessian is *strictly* $H^{1/2}(\Gamma)$-coercive at the optimal domain $\Omega^\star$. Since this is not the case as proven in the previous subsection, we cannot expect convergence of the solution of (1.22) to the solution $r^\star$ of the original shape optimization problem (1.1). This will be confirmed by our numerical results, see Section 3.

2. Numerical Method to compute the State and its Adjoint

2.1. **Reformulation of the State Equation.** The boundary value problems (1.2) and (1.4) have to be solved in each step of an iterative optimization process since the underlying domains are always different. Finite element methods suffer from generating a suitable triangulation for each new domain. One way out is to reformulate the given boundary value problems as boundary integral equations. This reformulation is managed by introducing a Newton potential N_f satisfying

$$-\Delta N_f = f \qquad \text{in } D \tag{2.23}$$

to resolve the inhomogenity in the state equation (1.2). This Newton potential is supposed to be explicitly known like in our numerical example (see Section 3) or computed with sufficiently high accuracy. We emphasize that the Newton potential has to be computed only once in advance.

Making the ansatz

$$u = N_f + v \tag{2.24}$$

yields then the problem of seeking a harmonic function v satisfying the following Dirichlet problem for the Laplacian

$$\begin{aligned} \Delta v &= 0 && \text{in } \Omega, \\ v &= g - N_f && \text{on } \Gamma. \end{aligned} \tag{2.25}$$

On the other hand, for computing the adjoint state p (cf. (1.4)), we make the ansatz

$$p = q + \chi_B(N_f - u_d).$$

Then, we are looking for the harmonic function q satisfying the following transmission problem

$$
\begin{aligned}
\Delta q &= 0 && \text{in } B,\\
[q] = N_f - u_d, \quad \left[\frac{\partial q}{\partial \mathbf{n}_\Sigma}\right] &= \frac{\partial (N_f - u)}{\partial \mathbf{n}_\Sigma} && \text{on } \Sigma,\\
\Delta q &= 0 && \text{in } \Omega \setminus \overline{B},\\
q &= 0 && \text{on } \Gamma.
\end{aligned} \tag{2.26}
$$

Now, we are able to compute both, the state and the adjoint state, by the method proposed in Subsection 2.3.

2.2. **Computing the Objective.** We shall show that it suffices to know the Cauchy data of the state and its adjoint on the boundaries Σ and Γ to compute both, the functional and the gradient. Being quite obvious in case of the shape gradient (1.3), this seems not to be true in case of the shape functional (1.1).

However, using the Gauß theorem we get

$$
\begin{aligned}
\int_B \langle \nabla u, \nabla u_d \rangle d\mathbf{x} &= \int_B u_d f \, d\mathbf{x} + \int_\Sigma u_d \frac{\partial u}{\partial \mathbf{n}_\Sigma} d\sigma_{\mathbf{x}},\\
\int_B \langle \nabla u, \nabla u \rangle d\mathbf{x} &= \int_B u f \, d\mathbf{x} + \int_\Sigma u \frac{\partial u}{\partial \mathbf{n}_\Sigma} d\sigma_{\mathbf{x}}.
\end{aligned}
$$

Employing next Greens's second formula for the state u and the Newton potential N_f gives

$$
\int_B u f \, d\mathbf{x} = \int_B f N_f \, d\mathbf{x} + \int_\Sigma N_f \frac{\partial u}{\partial \mathbf{n}_\Sigma} - u \frac{\partial N_f}{\partial \mathbf{n}_\Sigma} d\sigma_{\mathbf{x}}.
$$

Therefore, combining these identities, we conclude that

$$
\begin{aligned}
2J(\Omega) &= \int_B (N_f - 2u_d) f + \|\nabla u_d\|^2 \, d\mathbf{x} + \int_\Sigma u \frac{\partial (u - N_f)}{\partial \mathbf{n}_\Sigma} + (N_f - 2u_d) \frac{\partial u}{\partial \mathbf{n}_\Sigma} d\sigma_{\mathbf{x}}\\
&= C(B) + \int_\Sigma u \frac{\partial (u - N_f)}{\partial \mathbf{n}_\Sigma} + (N_f - 2u_d) \frac{\partial u}{\partial \mathbf{n}_\Sigma} d\sigma_{\mathbf{x}}.
\end{aligned} \tag{2.27}
$$

Herein, $C(B)$ is a constant independent from the actual domain Ω. Consequently, only the Cauchy data of the state at the fixed boundary Σ have to be computed to perform a line search.

2.3. **Boundary Integral Equations.** In view of (2.25) and (2.26) we shall provide a method to solve

$$
\begin{aligned}
\Delta u &= 0 && \text{in } B,\\
[u] = f, \quad \left[\frac{\partial u}{\partial \mathbf{n}_\Sigma}\right] &= g && \text{on } \Sigma,\\
\Delta u &= 0 && \text{in } \Omega \setminus \overline{B},\\
u &= h && \text{on } \Gamma,
\end{aligned} \tag{2.28}
$$

where we have to set $f, g = 0$ in case of (2.25).

For sake of convenience we assume in the sequel that $\mathbf{n}_\Sigma$ and $\mathbf{n}_\Gamma$ point inside $\Omega \setminus \overline{B}$. We introduce the *single layer operator* $\mathcal{V}_{\Phi\Psi}$, the *double layer operator* $\mathcal{K}_{\Phi\Psi}$, the *adjoint double layer operator* $\mathcal{K}^\star_{\Psi\Phi}$ and the *hypersingular operator* $\mathcal{W}_{\Phi\Psi}$ with respect to the boundaries $\Phi, \Psi \in \{\Gamma, \Sigma\}$ by

$$\left.\begin{aligned}
(\mathcal{V}_{\Phi\Psi}u)(\mathbf{x}) &:= \int_\Phi E(\mathbf{x},\mathbf{y})u(\mathbf{y})d\sigma_{\mathbf{y}},\\
(\mathcal{K}_{\Phi\Psi}u)(\mathbf{x}) &:= \int_\Phi \frac{\partial E(\mathbf{x},\mathbf{y})}{\partial \mathbf{n}_\Phi(\mathbf{y})}u(\mathbf{y})d\sigma_{\mathbf{y}},\\
(\mathcal{K}^\star_{\Phi\Psi}u)(\mathbf{x}) &:= \int_\Phi \frac{\partial E(\mathbf{x},\mathbf{y})}{\partial \mathbf{n}_\Psi(\mathbf{x})}u(\mathbf{y})d\sigma_{\mathbf{y}},\\
(\mathcal{W}_{\Phi\Psi}u)(\mathbf{x}) &:= -\frac{\partial}{\partial \mathbf{n}_\Psi(\mathbf{x})}\int_\Phi \frac{\partial E(\mathbf{x},\mathbf{y})}{\partial \mathbf{n}_\Phi(\mathbf{y})}u(\mathbf{y})d\sigma_{\mathbf{y}},
\end{aligned}\right\} \qquad \mathbf{x} \in \Psi,$$

where the fundamental solution $E(\mathbf{x},\mathbf{y})$ is defined as in (1.14). Notice that, in the present context, the operators with respect to one boundary are continuous mappings in terms of

$$\begin{aligned}
\mathcal{V}_{\Phi\Phi} &: H^{-1/2}(\Phi) \to H^{1/2}(\Phi), &\qquad \mathcal{W}_{\Phi\Phi} &: H^{1/2}(\Phi) \to H^{-1/2}(\Phi),\\
\mathcal{K}_{\Phi\Phi} &: H^{1/2}(\Phi) \to H^{1/2}(\Phi), &\qquad \mathcal{K}^\star_{\Phi\Phi} &: H^{-1/2}(\Phi) \to H^{-1/2}(\Phi),
\end{aligned}$$

while in the case of mixed boundaries the operators are arbitrarily smoothing compact operators.

Next, we introduce the variables $u_\Sigma = u|_\Sigma$, $\sigma_\Sigma := \partial u/\partial \mathbf{n}_\Sigma$, and $\sigma_\Gamma := \partial u/\partial \mathbf{n}_\Gamma$. Then, we find the following integral equations with respect to $u|_{\Omega\setminus\overline{B}}$

$$\begin{aligned}
\mathcal{W}_{\Sigma\Sigma}u_\Sigma + \mathcal{W}_{\Gamma\Sigma}h - \Big(\frac{1}{2} - \mathcal{K}^\star_{\Sigma\Sigma}\Big)\sigma_\Sigma + \mathcal{K}^\star_{\Gamma\Sigma}\sigma_\Gamma &= -\sigma_\Sigma &\qquad &\text{on } \Sigma,\\
\Big(\frac{1}{2} - \mathcal{K}_{\Sigma\Sigma}\Big)u_\Sigma - \mathcal{K}_{\Gamma\Sigma}h + \mathcal{V}_{\Sigma\Sigma}\sigma_\Sigma + \mathcal{V}_{\Gamma\Sigma}\sigma_\Gamma &= 0 &\qquad &\text{on } \Sigma,\\
-\mathcal{K}_{\Sigma\Gamma}u_\Sigma + \Big(\frac{1}{2} - \mathcal{K}_{\Gamma\Gamma}\Big)h + \mathcal{V}_{\Sigma\Gamma}\sigma_\Sigma + \mathcal{V}_{\Gamma\Gamma}\sigma_\Gamma &= 0 &\qquad &\text{on } \Gamma,
\end{aligned}$$

and with respect to $u|_B$

$$\begin{aligned}
\mathcal{W}_{\Sigma\Sigma}(u_\Sigma + f) + \Big(\frac{1}{2} + \mathcal{K}^\star_{\Sigma\Sigma}\Big)(\sigma_\Sigma + g) &= \sigma_\Sigma + g &\qquad &\text{on } \Sigma,\\
-\Big(\frac{1}{2} + \mathcal{K}_{\Sigma\Sigma}\Big)(u_\Sigma + f) + \mathcal{V}_{\Sigma\Sigma}(\sigma_\Sigma + g) &= 0 &\qquad &\text{on } \Sigma.
\end{aligned}$$

Adding the corresponding integral equations and rearranging the variables yields

$$\begin{aligned}
2\mathcal{W}_{\Sigma\Sigma}u_\Sigma + 2\mathcal{K}^\star_{\Sigma\Sigma}\sigma_\Sigma + \mathcal{K}^\star_{\Gamma\Sigma}\sigma_\Gamma &= -\mathcal{W}_{\Sigma\Sigma}f + \Big(\frac{1}{2} - \mathcal{K}^\star_{\Sigma\Sigma}\Big)g - \mathcal{W}_{\Gamma\Sigma}h &\qquad &\text{on } \Sigma,\\
-2\mathcal{K}_{\Sigma\Sigma}u_\Sigma + 2\mathcal{V}_{\Sigma\Sigma}\sigma_\Sigma + \mathcal{V}_{\Gamma\Sigma}\sigma_\Gamma &= \Big(\frac{1}{2} + \mathcal{K}_{\Sigma\Sigma}\Big)f - \mathcal{V}_{\Sigma\Sigma}g + \mathcal{K}_{\Gamma\Sigma}h &\qquad &\text{on } \Sigma,\\
-\mathcal{K}_{\Sigma\Gamma}u_\Sigma + \mathcal{V}_{\Sigma\Gamma}\sigma_\Sigma + \mathcal{V}_{\Gamma\Gamma}\sigma_\Gamma &= \Big(\mathcal{K}_{\Gamma\Gamma} - \frac{1}{2}\Big)h &\qquad &\text{on } \Gamma.
\end{aligned} \tag{2.29}$$

2.4. **The Variational Formulation.** Next, we introduce the product space $\mathcal{H} := H^{1/2}(\Sigma)\times H^{-1/2}(\Sigma) \times H^{-1/2}(\Gamma)$ equipped by the product norm

$$\|(u_\Sigma,\sigma_\Sigma,\sigma_\Gamma)\|_{\mathcal{H}}^2 := \|u_\Sigma\|_{H^{1/2}(\Sigma)}^2 + \|\sigma_\Sigma\|_{H^{-1/2}(\Sigma)}^2 + \|\sigma_\Gamma\|_{H^{-1/2}(\Gamma)}^2$$

for all $(u_\Sigma,\sigma_\Sigma,\sigma_\Gamma) \in \mathcal{H}$. Further, let $a : \mathcal{H}\times\mathcal{H} \to \mathbb{R}$, be the bilinear form defined by

$$\begin{aligned} &a\big((u_\Sigma,\sigma_\Sigma,\sigma_\Gamma),(v_\Sigma,\lambda_\Sigma,\lambda_\Gamma)\big) \\ &= \left(\begin{bmatrix} v_\Sigma \\ \lambda_\Sigma \\ \lambda_\Gamma \end{bmatrix}, \begin{bmatrix} 2\mathcal{W}_{\Sigma\Sigma} & 2\mathcal{K}^\star_{\Sigma\Sigma} & \mathcal{K}^\star_{\Gamma\Sigma} \\ -2\mathcal{K}_{\Sigma\Sigma} & 2\mathcal{V}_{\Sigma\Sigma} & \mathcal{V}_{\Gamma\Sigma} \\ -\mathcal{K}_{\Sigma\Gamma} & \mathcal{V}_{\Sigma\Gamma} & \mathcal{V}_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} u_\Sigma \\ \sigma_\Sigma \\ \sigma_\Gamma \end{bmatrix}\right)_{L^2(\Sigma)\times L^2(\Sigma)\times L^2(\Gamma)}. \end{aligned} \tag{2.30}$$

Introducing the linear functional $F : \mathcal{H} \to \mathbb{R}$,

$$\begin{aligned} &F(v_\Sigma,\lambda_\Sigma,\lambda_\Gamma) \\ &= \left(\begin{bmatrix} v_\Sigma \\ \lambda_\Sigma \\ \lambda_\Gamma \end{bmatrix}, \begin{bmatrix} -\mathcal{W}_{\Sigma\Sigma} & 1/2-\mathcal{K}^\star_{\Sigma\Sigma} & -\mathcal{W}_{\Gamma\Sigma} \\ 1/2+\mathcal{K}_{\Sigma\Sigma} & -\mathcal{V}_{\Sigma\Sigma} & \mathcal{K}_{\Gamma\Sigma} \\ 0 & 0 & \mathcal{K}_{\Gamma\Gamma}-1/2 \end{bmatrix} \begin{bmatrix} f \\ g \\ h \end{bmatrix}\right)_{L^2(\Sigma)\times L^2(\Sigma)\times L^2(\Gamma)} \end{aligned} \tag{2.31}$$

the variational formulation is given by:

Seek $(u_\Sigma,\sigma_\Sigma,\Sigma_\Gamma) \in \mathcal{H}$ such that

$$a\big((u_\Sigma,\sigma_\Sigma,\sigma_\Gamma),(v_\Sigma,\lambda_\Sigma,\lambda_\Gamma)\big) = F(v_\Sigma,\lambda_\Sigma,\lambda_\Gamma) \tag{2.32}$$

for all $(v_\Sigma,\lambda_\Sigma,\lambda_\Gamma) \in \mathcal{H}$.

Lemma 2.1. *The bilinear form $a(\cdot,\cdot)$ from (2.30) satisfies the Gårding inequality*

$$a\big((u_\Sigma,\sigma_\Sigma,\sigma_\Gamma),(v_\Sigma,\sigma_\Sigma,\sigma_\Gamma)\big) + \|u_\Sigma\|_{L^2(\Sigma)}^2 \gtrsim \|(u_\Sigma,\sigma_\Sigma,\sigma_\Gamma)\|_{\mathcal{H}}^2, \tag{2.33}$$

provided that Ω has a conformal radius < 1 if $n = 2$.

Proof. From $\mathcal{K}_{\Phi\Psi} = \mathcal{K}^\star_{\Psi\Phi}$ we conclude $(\mathcal{K}_{\Phi\Psi}\sigma_\Phi,\sigma_\Psi)_{L^2(\Psi)} = (\mathcal{K}^\star_{\Psi\Phi}\sigma_\Psi,\sigma_\Phi)_{L^2(\Phi)}$. Hence, we arrive at

$$\begin{aligned} &a\big((u_\Sigma,\sigma_\Sigma,\sigma_\Gamma),(u_\Sigma,\sigma_\Sigma,\sigma_\Gamma)\big) \\ &\quad = 2(\mathcal{W}_{\Sigma\Sigma}u_\Sigma,u_\Sigma)_{L^2(\Sigma)} + \left(\begin{bmatrix} \sigma_\Sigma \\ \sigma_\Gamma \end{bmatrix}, \begin{bmatrix} 2\mathcal{V}_{\Sigma\Sigma} & \mathcal{V}_{\Gamma\Sigma} \\ \mathcal{V}_{\Sigma\Gamma} & \mathcal{V}_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} \sigma_\Sigma \\ \sigma_\Gamma \end{bmatrix}\right)_{L^2(\Sigma)\times L(\Gamma)}, \end{aligned}$$

Observing that the operator

$$\widetilde{\mathcal{V}} : H^{-1/2}(\Sigma)\times H^{-1/2}(\Gamma) \to H^{1/2}(\Sigma)\times H^{1/2}(\Gamma), \qquad \widetilde{\mathcal{V}} := \begin{bmatrix} 2\mathcal{V}_{\Sigma\Sigma} & \mathcal{V}_{\Gamma\Sigma} \\ \mathcal{V}_{\Sigma\Gamma} & \mathcal{V}_{\Gamma\Gamma} \end{bmatrix},$$

is positive definite, we deduce the assertion since

$$(\mathcal{W}_{\Sigma\Sigma}u_\Sigma,u_\Sigma)_{L^2(\Sigma)} \gtrsim |u_\Sigma|_{H^{1/2}(\Sigma)}^2$$

for all $u_\Sigma \in H^{1/2}(\Omega)$.

□

Lemma 2.2. *The bilinear form $a(\cdot,\cdot)$ from (2.30) is injective, provided that Ω has a conformal radius < 1 if $n = 2$.*

Proof. Assume that $(u_\Sigma^{(1)}, \sigma_\Sigma^{(1)}, \sigma_\Gamma^{(1)}), (u_\Sigma^{(2)}, \sigma_\Sigma^{(2)}, \sigma_\Gamma^{(2)}) \in \mathcal{H}$ solve both the transmission problem (2.28). Then, setting $(v_\Sigma, \lambda_\Sigma, \lambda_\Gamma) := (u_\Sigma^{(1)} - u_\Sigma^{(1)}, \sigma_\Sigma^{(1)} - \sigma_\Sigma^{(2)}, \sigma_\Gamma^{(1)} - \sigma_\Gamma^{(2)}) \in \mathcal{H}$, the Gårding inequality (2.1) implies $v_\Sigma = const.$ and $\lambda_\Sigma = \lambda_\Gamma = 0$. Since the underlying function is harmonic in Ω and satisfies homogeneous Dirichlet boundary conditions at Γ, it follows that $const. = 0$. $\square$

Combining Lemmata 2.1 and 2.2 yields the following theorem.

Theorem 2.3. *The variational formulation (2.32) admits a unique solution $(u_\Sigma, \sigma_\Sigma, \sigma_\Gamma) \in \mathcal{H}$ for all $F \in \mathcal{H}'$, provided that Ω has a conformal radius < 1 if $n = 2$.*

Proof. The bilinear form $a(\cdot,\cdot)$ is obviously continuous on $\mathcal{H} \times \mathcal{H}$ and in accordance with Lemmata 2.1 and 2.2 $\mathcal{H}$-coercive and injective. Hence, one concludes existence and uniqueness of the solution by the Riesz-Schauder theory. $\square$

2.5. **The Galerkin Discretization.** Since the variational formulation is stable without further restrictions, it suffices to exploit globally continuous piecewise linear or bilinear ansatz functions to discretize u_Σ and piecewise constant ansatz functions to discretize σ_Σ and σ_Γ. To this end, we introduce suitable triangulations of the boundaries Σ and Γ, which we suppose to have similar mesh sizes. For the Dirichlet data we introduce canonical globally continuous piecewise linear (or bilinear) ansatz functions $\{\phi_k^\Phi : k \in \Delta^\Phi\}$. For the Neumann data we consider canonical piecewise constant ansatz functions $\{\psi_k^\Phi : k \in \nabla^\Phi\}$ on the given triangulations of the boundaries Φ ($\Phi \in \{\Sigma, \Gamma\}$). Note that $\#\Delta^\Phi \sim \#\nabla^\Psi$, $\Phi, \Psi \in \{\Sigma, \Gamma\}$.

Then, introducing the system matrices

$$
\begin{aligned}
\mathbf{W}_{\Phi\Psi} &= \Big[(\mathcal{W}_{\Phi\Psi}\phi_\ell^\Phi, \phi_k^\Psi)_{L^2(\Psi)}\Big]_{k,\ell}, & \mathbf{G}_\Phi &= \Big[(\phi_\ell^\Phi, \phi_k^\Phi)_{L^2(\Phi)}\Big]_{k,\ell},\\
\mathbf{K}_{\Phi\Psi} &= \Big[(\mathcal{K}_{\Phi\Psi}\phi_\ell^\Phi, \psi_k^\Psi)_{L^2(\Psi)}\Big]_{k,\ell}, & \mathbf{B}_\Phi &= \Big[\tfrac{1}{2}(\phi_\ell^\Phi, \psi_k^\Phi)_{L^2(\Phi)}\Big]_{k,\ell},\\
\mathbf{V}_{\Phi\Psi} &= \Big[(\mathcal{V}_{\Phi\Psi}\psi_\ell^\Phi, \psi_k^\Psi)_{L^2(\Psi)}\Big]_{k,\ell}, & \mathbf{H}_\Phi &= \Big[(\psi_\ell^\Phi, \psi_k^\Phi)_{L^2(\Phi)}\Big]_{k,\ell},
\end{aligned}
\tag{2.34}
$$

where again $\Phi, \Psi \in \{\Sigma, \Gamma\}$, and the data vectors

$$
\mathbf{f} = \Big[(f, \psi_k^\Sigma)_{L^2(\Sigma)}\Big]_k, \qquad \mathbf{g} = \Big[(g, \phi_k^\Sigma)_{L^2(\Sigma)}\Big]_k, \qquad \mathbf{h} = \Big[(h, \phi_k^\Gamma)_{L^2(\Gamma)}\Big]_k,
$$

we obtain the following linear system of equations

$$
\begin{bmatrix} 2\mathbf{W}_{\Sigma\Sigma} & 2\mathbf{K}_{\Sigma\Sigma}^\star & \mathbf{K}_{\Sigma\Gamma}^\star \\ -2\mathbf{K}_{\Sigma\Sigma} & 2\mathbf{V}_{\Sigma\Sigma} & \mathbf{V}_{\Gamma\Sigma} \\ -\mathbf{K}_{\Sigma\Gamma} & \mathbf{V}_{\Sigma\Gamma} & \mathbf{V}_{\Gamma\Gamma} \end{bmatrix}
\begin{bmatrix} \mathbf{u}_\Sigma \\ \boldsymbol{\sigma}_\Sigma \\ \boldsymbol{\sigma}_\Gamma \end{bmatrix}
=
\begin{bmatrix} -\mathbf{W}_{\Sigma\Sigma} & \mathbf{K}_{\Sigma\Sigma}^\star - \mathbf{B}_\Sigma^\star & -\mathbf{W}_{\Gamma\Sigma} \\ \mathbf{K}_{\Sigma\Sigma} + \mathbf{B}_\Sigma & \mathbf{V}_{\Sigma\Sigma} & \mathbf{K}_{\Gamma\Sigma} \\ \mathbf{0} & \mathbf{0} & \mathbf{K}_{\Gamma\Gamma} - \mathbf{B}_\Gamma \end{bmatrix}
\begin{bmatrix} \mathbf{H}_\Sigma^{-1}\mathbf{f} \\ \mathbf{G}_\Sigma^{-1}\mathbf{g} \\ \mathbf{G}_\Gamma^{-1}\mathbf{h} \end{bmatrix}
\tag{2.35}
$$

We mention that $\mathbf{H}_\Sigma^{-1}\mathbf{f}$ and $\mathbf{G}_\Sigma^{-1}\mathbf{g}, \mathbf{G}_\Gamma^{-1}\mathbf{h}$ correspond to the L^2-orthogonal projections of the given data $f \in H^{-1/2}(\Sigma)$ and $g \in H^{1/2}(\Sigma), h \in H^{1/2}(\Gamma)$ onto the assciated spaces of the piecewise constants and (bi-) linears. That way, we can apply fast boundary element techniques also to the boundary integral operators on the right hand side of the arising linear system of equations (2.35).

Applying standard error estimates for the Galerkin scheme and employing the Aubin-Nitsche trick leads to the following error estimate concerning the present discretization.

Proposition 2.4. *Let h denote the mesh size of the triangulations of Σ and Γ, respectively. We denote the solution of (2.32) by $(u_\Sigma, \sigma_\Sigma, \sigma_\Sigma)$ and the Galerkin solution by $(u_\Sigma^h, \sigma_\Sigma^h, \sigma_\Gamma^h)$. Then, we have the error estimate*

$$\begin{aligned}\|(u, \sigma_\Sigma, \sigma_\Gamma) - (u^h, \sigma_\Sigma^h, \sigma_\Gamma^h)\|_{H^{-1}(\Sigma)\times H^{-2}(\Sigma)\times H^{-2}(\Sigma)}& \\ \lesssim h^3\big\{\|u_\Sigma\|_{H^2(\Sigma)} + \|\sigma_\Sigma\|_{H^1(\Gamma)} + \|\sigma_\Gamma\|_{H^1(\Gamma)}\big\}&\end{aligned}$$

uniformly in h.

Finally, we shall encounter some issues on the efficient solution of the linear system of equations (2.35). The complexity of computing the solution is at least quadratically since the system matrices are densely populated. Applying fast boundary element techniques the complexity can be reduced considerably. We use wavelet matrix compression ([4, 16, 27]) which yields in combination with the wavelet preconditioning ([5]) to a numerical scheme of linear over-all complexity without compromising stability and accuracy of the underlying Galerkin scheme.

2.6. **Error Estimates.** Recall that, in a single iteration step of the shape optimization algorithm, we use the present method in order to solve both, (2.25) to compute the state via (2.24) and (1.4) to compute the adjoint state. Now, we shall specify the approximation errors to the shape functional and its gradient. For sake of simplicity we neglect approximation errors of the Newton potential N_f (2.23), i.e., we assume that it is known analytically.

Corollary 2.5. *Assume that the Newton potential N_f from (2.23) is given exactly. Then, the shape functional converges cubically and the shape gradient converges quadratically, that is, the approximation errors behave like $\mathcal{O}(h^3)$ and $\mathcal{O}(h^2)$, respectively.*

Proof. In accordance with (2.27) we find

$$2|J(\Omega) - J^h(\Omega)| = \left|\int_\Sigma (u_\Sigma\sigma_\Sigma - u_\Sigma^h\sigma_\Sigma^h) - (u_\Sigma - u_\Sigma^h)\frac{\partial N_f}{\partial \mathbf{n}_\Sigma} + (N_f - 2u_d)(\sigma_\Sigma - \sigma_\Sigma^h) d\sigma_{\mathbf{x}}\right|.$$

Due to

$$u_\Sigma\sigma_\Sigma - u_\Sigma^h\sigma_\Sigma^h = (u_\Sigma^h - u_\Sigma)(\sigma_\Sigma - \sigma_\Sigma^h) + u_\Sigma(\sigma_\Sigma - \sigma_\Sigma^h) + \sigma_\Sigma(u_\Sigma - u_\Sigma^h)$$

we can estimate the first term by

$$\begin{aligned}\left|\int_\Sigma (u_\Sigma\sigma_\Sigma - u_\Sigma^h\sigma_\Sigma^h) d\sigma_{\mathbf{x}}\right| &\le \|u_\Sigma^h - u_\Sigma\|_{L^2(\Sigma)}\|\sigma_\Sigma - \sigma_\Sigma^h\|_{L^2(\Sigma)} \\ &+ \|u_\Sigma\|_{H^2(\Sigma)}\|\sigma_\Sigma - \sigma_\Sigma^h\|_{H^{-2}(\Sigma)} + \|\sigma_\Sigma\|_{H^1(\Sigma)}\|u_\Sigma - u_\Sigma^h\|_{H^{-1}(\Sigma)} = \mathcal{O}(h^3).\end{aligned}$$

Further, we find

$$\left|\int_\Sigma (u_\Sigma - u_\Sigma^h)\frac{\partial N_f}{\partial \mathbf{n}_\Sigma} d\sigma_{\mathbf{x}}\right| \le \|u_\Sigma - u_\Sigma^h\|_{H^{-1}(\Sigma)} \left\|\frac{\partial N_f}{\partial \mathbf{n}_\Sigma}\right\|_{H^1(\Sigma)} = \mathcal{O}(h^3),$$

$$\left|\int_\Sigma (N_f - 2u_d)(\sigma_\Sigma - \sigma_\Sigma^h) d\sigma_{\mathbf{x}}\right| \le \|\sigma_\Sigma - \sigma_\Sigma^h\|_{H^{-2}(\Sigma)} \|N_f - 2u_d\|_{H^2(\Sigma)} = \mathcal{O}(h^3),$$

which shows $|J(\Omega) - J_h(\Omega)| = \mathcal{O}(h^3)$.

For sake of convenience we set $\sigma_\Gamma := \partial(u-g)/\partial \mathbf{n}_\Gamma$ and $\lambda_\Gamma := \partial p/\partial \mathbf{n}_\Gamma$, while σ_Γ^h and λ_Γ^h denote the numerical approximations. Likewise to above, we conclude

$$\begin{aligned}
|\nabla J(\Omega)[dr] - \nabla J^h(\Omega)[dr]| &= \left|\int_\Gamma \langle \mathbf{V}, \mathbf{n}\rangle \big\{\sigma_\Gamma \lambda_\Gamma - \sigma_\Gamma^h \lambda_\Gamma^h\big\} d\sigma\right| \\
&= \left|\int_\Gamma \langle \mathbf{V}, \mathbf{n}\rangle \big\{(\sigma_\Gamma^h - \sigma_\Gamma)(\lambda_\Gamma - \lambda_\Gamma^h) - \sigma_\Gamma(\lambda_\Gamma - \lambda_\Gamma^h) - \lambda_\Gamma(\sigma_\Gamma - \sigma_\Gamma^h)\big\} d\sigma\right| \\
&\le \|\langle \mathbf{V}, \mathbf{n}\rangle\|_{L^\infty(\Gamma)} (|\sigma_\Gamma - \sigma_\Gamma^h|, |\lambda_\Gamma - \lambda_\Gamma^h|)_{L^2(\Gamma)} + (\langle \mathbf{V}, \mathbf{n}\rangle \sigma_\Gamma, \lambda_\Gamma - \lambda_\Gamma^h)_{L^2(\Gamma)} \\
&\qquad + (\langle \mathbf{V}, \mathbf{n}\rangle \lambda_\Gamma, \sigma_\Gamma - \sigma_\Gamma^h)_{L^2(\Gamma)}.
\end{aligned}$$

Herein, the first term is estimated by

$$(|\sigma_\Gamma - \sigma_\Gamma^h|, |\lambda_\Gamma - \lambda_\Gamma^h|)_{L^2(\Gamma)} \le \|\sigma_\Gamma - \sigma_\Gamma^h\|_{L^2(\Gamma)} \|\lambda_\Gamma - \lambda_\Gamma^h\|_{L^2(\Gamma)} = \mathcal{O}(h^2).$$

The second term yields

$$(\langle \mathbf{V}, \mathbf{n}\rangle \sigma_\Gamma, \lambda_\Gamma - \lambda_\Gamma^h)_{L^2(\Gamma)} \le \|\langle \mathbf{V}, \mathbf{n}\rangle \sigma_\Gamma\|_{H^1(\Gamma)} \|\lambda_\Gamma - \lambda_\Gamma^h\|_{H^{-1}(\Gamma)} = \mathcal{O}(h^2),$$

and similarly the third term, which finishes the proof. □

3. Numerical Results

The numerical example will be carried out in two space dimensions. Let B be the circle $\{(x,y) : x^2 + y^2 < 0.2\}$ and

$$E_z := \big\{(x,y) \in \mathbb{R}^2 : x^2 + 4y^2 < z^2\big\}, \quad z > 0.2,$$

denote the ellipse with semi-axes $h_x = z$ and $h_y = z/2$. The function u is supposed to satisfy the Poisson equation $-\Delta u = f = 10$ in Ω with homogeneous Dirichlet data $u|_\Gamma = g = 0$. The function u_d is chosen as $u_d(x,y) := 1 - x^2 - 4y^2$. Similar to Example 1.4, we infer $J(E_z) = 0$ for all $z > 0.2$ and thus all ellipses E_z are minimizers of the problem under consideration. For the present state equation we will exploit the Newton potential $N_f = -5(x^2 + y^2)/2$.

First, we shall check the orders of convergence predicted in Corollary 2.5. We compute the shape functional and its discretized gradient in case of the ellipse with semi-axis $h_x = 0.4$ and $h_y = 0.6$ on a very fine discretization. Then, we compute on lower levels the approximate solutions und measure the absolute (ℓ^2-) errors to our reference values. The results are depicted in Figure 3.2. In fact, one observes cubic and quadratic approximation orders (indicated by the dashed lines) of the functional and its gradient, respectively. Hence, difficulties in the numerical optimization tests are *not* caused by lack of accuracy.

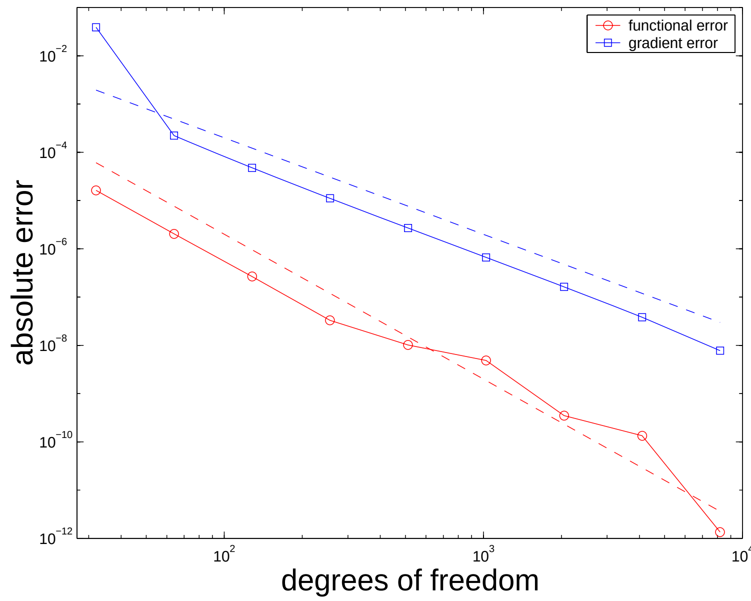

FIGURE 3.2. Degrees of freedom versus approximation error.

Next, we try to find the unknown boundary by standard optimization methods. To ensure uniqueness for the problem under consideration, the canonical idea is the use of the complete $H^1(B)$-norm of the state, i.e., looking at

$$J(\Omega) = \frac{1}{2}\int_B \big(u(\mathbf{x}) - u_d(\mathbf{x})\big)^2 + \|\nabla u(\mathbf{x}) - \nabla u_d(\mathbf{x})\|^2 d\mathbf{x} \to \inf .$$

However, since potential values itself have no meaning for applications in both, fluid dynamics and magnetostatics, we introduce instead an additional volume constraint

$$V(\Omega) = \int_\Omega d\mathbf{x} = V_0,$$

as it was already proposed by Mohammadi and Pironneau in [22]. We compute an approximation for the unknown boundary Γ in case of $V_0 = 0.25^2 \cdot 2\pi$, $0.3^2 \cdot 2\pi$, $0.35^2 \cdot 2\pi$, $0.4^2 \cdot 2\pi$ by using the first 33 Fourier frequencies and 1024 piecewise constant and linear boundary elements per boundary, respectively. The constraint optimization problem is treated by an Augmented Lagrangian. The descent direction is derived from a quasi-Newton method with quadratic line search, updated by the inverse BFGS-rule without damping, see e.g. [13, 14] for the details. We choose always the circle centered in $(x, y) = (0, 0)$ with volume V_0 as initial guess and perform 100 quasi-Newton iterations. The resulting free boundaries are plotted in Figure 3.3. The inner boundary corresponds to the problem with $V_0 = 0.25^2 \cdot 2\pi$ while the outer boundary corresponds to $V_0 = 0.4^2 \cdot 2\pi$. Especially, we observe that the computed free boundaries are only approximately the correct ellipses since oscillations occur. Indeed, a regularization in terms of a certain $H^s(\Gamma)$-norm can be applied, as it is proposed in principle by Mohammadi and Pironneau in [23]. According

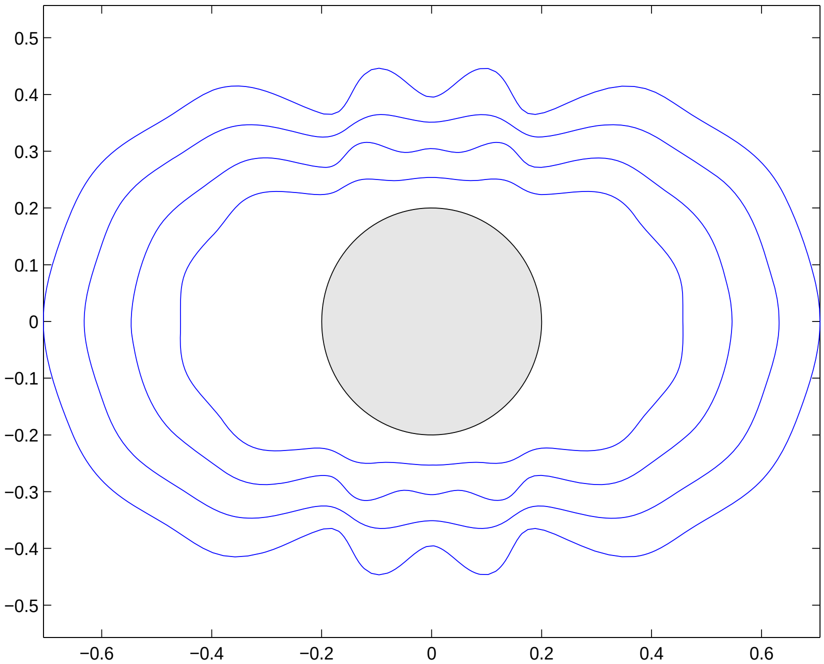

FIGURE 3.3. Computed free boundaries.

to the nature of the shape Hessian of the original objective, the space $H^{1/2}(\Gamma)$ seems to be convenient from our point of view.

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